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Calculation of the temperature field of the material in the thermal model of laser ablation

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Abstract. The mechanisms of laser ablation of materials under the interaction of powerful pulsed laser radiation with a material coated with a thin film system were studied. One of the first models of such interaction of high-power laser radiation with matter was the thermal model. A one-temperature thermal model was used when considering the interaction of laser radiation with dielectrics, and a two-temperature model was used when considering the interaction of laser radiation with metals. When studying the processes of laser ablation within the framework of the thermal model, the method of moments with a special selection of the test function was chosen. Computer simulation was conducted to study the dependence of the surface temperature and the characteristic thermal length on the radiant flux. Variants with both constant and variable optophysical characteristics of the phenomenon were considered. Calculations were performed for different time ranges under different initial conditions. The results of the numerical experiment agree well with the data of other authors.

1 Introduction

Composite materials based on ceramics and glasses are widely used, for example, in optoelectronics, nanophotonics [1–7]. The task of interaction of such composite materials under irradiation conditions with powerful pulses of laser radiation are important [8–12]. Such tasks associated with laser-induced destruction of optical materials require the ability to determine the strength and reliability of the irradiated material and predict the dynamics of the temperature field in the irradiated substance, and the forming vapor-plasma plume produced by laser ablation. The interaction of laser radiation with material causes a number of physical and chemical processes in the irradiated material: optical, thermal and mechanical [13–16]. Among these processes, we distinguish processes of material destruction, including laser ablation with the formation of craters and/or cracking of the material surface [17–22].

In this research, the results of a theoretical study of the effect of high-power pulsed laser radiation on materials were considered [23–32]. The aim of the research is to compare the known calculation procedures of the temperature field when a material is irradiated with short laser pulses. When considering laser ablation destruction, the authors used the thermal model [33, 34]. The results of a numerical solution of the nonstationary heat conduction equation by the method of moments are presented.

2 Thermal model

It is possible to distinguish, in the general case, three characteristic regions in the interaction of high-power laser radiation with a material: a vapor-plasma plume, a liquid melt, and a solid material. Consider the dynamics of the temperature field in a base solid material.

When considering the temperature field in a medium [18, 19, 35–38], the heat conduction equations for dielectrics were solved in the framework of a one-temperature model

$$c\frac{\partial T}{\partial t}=\nabla\cdot\left(\kappa\nabla T\right)+S, \tag{1}$$

and for metals in the framework of a two-temperature model

$$c_e\frac{\partial T_e}{\partial t}=\nabla\cdot\left(\kappa_e\nabla T_e\right)-G_{ep}(T_e-T_i)+S, \tag{2}$$

$$c_i\frac{\partial T_i}{\partial t}=\nabla\cdot\left(\kappa_i\nabla T_i\right)+G_{ep}(T_e-T_i), \tag{3}$$

where c, κ is the heat capacity and thermal conductivity of the dielectric material, T is the temperature of its surface, $S = S(\mathbf{r}, t)$ is the function describing the heat source, in this case the part of the energy of the laser pulse absorbed by the material at the point with the radius-vector $\mathbf{r}$, the quantities describing parameters of the electron cloud and lattice ions (phonon cloud) are denoted by the indices e and i, respectively, G_{ep} is the coefficient establishing the rate of energy exchange between electrons and phonons.

Since the size of the region to be destroyed and heated is often much smaller than the size of the irradiation spot on the surface of the material, equations (1)–(3) are considered in a one-dimensional version by the most of authors. The numerical solution of these equations by the authors [19–21, 33, 34] was carried out by the method of moments and made it possible to determine the dynamics of propagation of the temperature field in the irradiated material over time, i.e. functional dependence of the form $T(t)$.

To verify the obtained results, comparisons were made with known analytical or empirical data [19]. Thus, for femtosecond pulses

$$T_e=\sqrt{T_0^2+2\frac{I_a\alpha}{C_e}t\exp\left(-\alpha z\right)}, \tag{4}$$

where T_0 is the initial temperature of the surface, $I_a = (1 - R)I_0$, the intensity of the absorbed laser radiation, $C_e = c_eT_e$ is assumed to be constant, see for example [39] and references therein. At the end of the pulse τ_L, the temperature of the electrons is

$$T_e=\sqrt{2\frac{I_a\alpha}{C_e}\tau_L\exp\left(-\frac{\alpha z}{2}\right)}, \tag{5}$$

and after the termination of the pulse, the temperature of the lattice ions is calculated from formula

$$T_i = \frac{I_a \alpha}{C_e} \tau_L \exp(-\alpha z). \qquad (6)$$

For picosecond pulses $\tau_e << \tau_L << \tau_i$ and for $t >> \tau_e$, the authors of [39] suggest the following approximation

$$T_i = T_0 + \frac{1}{\tau_i} \int_0^t \exp\left(-\frac{t-t^*}{\tau_i}\right) T_e dt^*, \qquad (7)$$

and for $t << \tau_i$ the formula is

$$T_i = T_e \left[1 - \exp\left(-\frac{t}{\tau_i}\right)\right] \approx \frac{t}{\tau_i} T_e. \qquad (8)$$

With certain additional simplifications after termination of the laser pulse, the formulas for the temperature of the electron cloud and the lattice ions are [39]:

$$T_e = \frac{I_a \alpha}{G_{ep}} \exp(-\alpha z), \quad T_i = \frac{I_a \alpha}{C_i} \tau_L \exp(-\alpha z). \qquad (9)$$

3 The method of moments

The authors of [23–32] carried out research of various materials, including dielectrics and metals. The results of one calculation for metals are shown here. The dynamics of a laser pulse with time was modeled by the expression

$$I = I_0 \frac{t}{\tau_L} \exp\left(-\frac{t}{\tau_L}\right), \qquad (10)$$

where $I_0 = 15 \cdot 10^{10}$ J·cm^{-2}·s^{-1} is the intensity of laser radiation and $\tau_L = 1$ ps is the pulse duration.

For the numerical solution of the obtained one-dimensional heat conduction equations, the method of moments was used [19]. In this case for a two-temperature model trial function, as in [19], was taken in the form

$$T_e = \frac{1}{1-\alpha l_e}\left[(T_{eS} + k)\exp(-\alpha z) - (\alpha l_e T_{eS} + k)\exp\left(-\frac{z}{l_e}\right)\right], \qquad (11)$$

$$T_i = \frac{1}{1-\alpha l_i}\left[(T_{iS} + k)\exp(-\alpha z) - (\alpha l_i T_{iS} + k)\exp\left(-\frac{z}{l_i}\right)\right], \qquad (12)$$

where the second term in parentheses had the form $k = \frac{J_e l_e}{\kappa_e}$ and $k = \frac{J_i l_i}{\kappa_i}$ for the electron and ion clouds, respectively.

Applying the moment method [33], the system of nonlinear partial derivatives equations (2), (3) is replaced by a system of homogeneous first-order differential equations for the functions $T_S(t)$ and $l(t)$, which in matrix form are

$$\mathbf{MN} = \mathbf{X}, \tag{13}$$

where

$$\mathbf{M}_{44} = \begin{pmatrix} m_{11} & \dots & m_{14} \\ \dots & \dots & \dots \\ m_{41} & \dots & m_{44} \end{pmatrix}, \quad \mathbf{X} = \begin{pmatrix} \dot{T}_e \\ \dot{T}_i \\ \dot{l}_e \\ \dot{l}_i \end{pmatrix}, \quad \mathbf{N} = \begin{pmatrix} n_1 \\ \dots \\ n_4 \end{pmatrix}. \tag{14}$$

The numerical solution of the system (13) was carried out with the help of the corresponding mathematical software, the MATLAB software package. The results of calculations of the surface temperature dynamics for the values of the parameters taken from [19] are shown in Fig. 1. In this figure, our results are shown in thick lines. The solid line shows the temperature of the electron cloud on the irradiated surface, the dashed line shows the phonon cloud on the same surface. For comparison, in the same figure, the results of similar calculations of the authors [19] are shown in thin lines.

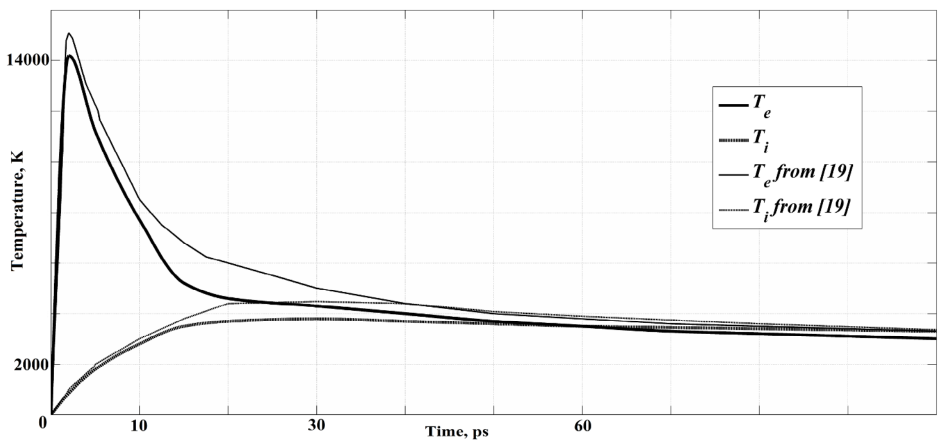

Fig. 1. Dynamics of metal heating by a laser pulse. Notations are in the text.

It can be considered that a qualitative coincidence has been achieved and good quantitative agreement in the results has been obtained. In this case, in the research of the authors, a maximum temperature of an electron cloud of 14200 K and an ion cloud of 3800 K is reached at 1.8 ps and 30 ps, respectively. In [19], the maximum temperature of the electron cloud of 15100 K and the ion cloud of 4400 K is reached at time points of 1.8 ps and 29 ps, respectively. Such a coincidence of results can be considered good. A slight discrepancy in the dynamics of the temperature field curves and their values can be attributed to the difference in the numerical method, with the aid of which the resulting system of ordinary differential equations was solved.

4 Conclusions

Thus, laser ablation destruction of materials using a thermal model has been studied. The numerical solution was carried out using the method of moments, one of the varieties of projection-grid methods for solving differential equations.

The developed algorithm of the solution and the created software allow to analyze the dynamics of a number of parameters of laser ablation destruction – surface temperature, thermal length, thickness of the ablated layer, ablation rate, – taking into account the different functional dependence of the thermophysical parameters of the initial system of heat conduction equations, including nonlinear edge conditions that may depend both on the time, and on the coordinate in an arbitrary way.

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